

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.74e-10 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.85e-01

Confidence level: 2.63e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Buminafos [ISO]</div> <div>Measured: 2.30e-11</div> <div>Predicted: 3.69e-04</div>	<div>Image not found</div> <div>Sulcotrione</div> <div>Measured: 1.73e-08</div> <div>Predicted: 2.68e-08</div>	<div>Image not found</div> <div>MCPB ethyl</div> <div>Measured: 7.50e-10</div> <div>Predicted: 1.69e-05</div>
<div>Image not found</div> <div>Oct-2-yne</div> <div>Measured: 5.00e-11</div> <div>Predicted: 10.3</div>	<div>Image not found</div> <div>3-Methyl-N-phenylaniline</div> <div>Measured: 1.79e-11</div> <div>Predicted: 1.24e-04</div>	